News and Views

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Biocomposites: Using light to drive biosynthesis

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Immobilization of membrane-bound proteins in inorganic matrices could allow creation of materials capable of mimicking biological processes. Advances in sol–gel biocomposites have now allowed development of a material that can use light to drive biosynthesis of ATP.

Membrane receptor proteins are the gatekeepers of the cell, and play a critical role in controlling cellular processes. Receptors such as ion channels are responsible for initiation of transmembrane signals, and can be used to control a variety of downstream biochemical processes. The immobilization of active membrane-bound receptors in inorganic matrices is a critical step in harnessing the potential of such biological processes for the development of improved biologically active materials. However, the need to maintain membrane integrity during immobilization generally renders membrane receptors less stable than soluble proteins such as antibodies and enzymes, and thus such species are difficult to immobilize in an active form. Bruce Dunn and colleagues at the University of California, Los Angeles have made an important step forward by demonstrating that sol–gel-derived materials can be used to entrap membrane-bound proteins in a physiologically active form[1]. The researchers use the new biocomposite materials for light-driven proton pumping and biosynthesis of ATP.

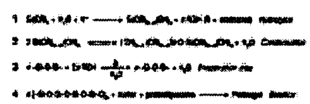
The immobilization of membrane receptors has traditionally been done by fusing liposomes containing the receptor of interest with a suitably derivatized surface. Examples include immobilization on thiolipid-modified

gold surfaces[2] or artificial immobilized membranes[3]. However, such methods tend to result in a situation where the interior aqueous compartment of the liposome is replaced by a solid surface, thus eliminating the ability to establish transmembrane ion gradients.

The entrapment of biological species within sol–gel-derived silica was first demonstrated[4] in the early 1990s, and spawned a vigorous field of research. The basic process involves using liquid silane precursors, such as tetra-alkoxysilanes, as precursors to silica. Hydrolysis of such precursors under acidic or basic conditions, followed by condensation of the resulting silane species in the presence of a buffered solution of protein, leads to a porous protein-doped silica material that allows passage of small molecules through the matrix while retaining the larger proteins (Fig. 1). Entrapment of a wide variety of soluble proteins in sol–gel-derived silica has been reported[5], and this method has proved capable of maintaining protein activity over periods of months or more.

Fig. 1

Figure 1 | **Example of the biocompatible sol–gel processing method used to entrap proteoliposomes into silica materials.**



Although soluble protein entrapment is for the most part relatively straightforward, immobilization of membrane-bound proteins has proved to be much more problematic. In part, this is due to the detrimental effects of the alcohol side-products of alkoxysilane hydrolysis, which can disrupt membrane structure[6] and thus deactivate the membrane proteins. The recent emergence of biocompatible sol–gel precursors, such as glyceroxysilanes[7], and biocompatible processing methods, including rotary evaporation of alkoxysilane sols before introduction of protein[8], have seen a revival of studies involving entrapment of membrane-bound proteins. Using such processing conditions, sometimes in conjunction with polymers to alter the porosity of the resulting material, transmembrane peptides such as gramicidin A (ref. 9), and receptors such as the acetylcholine receptor and dopamine receptor[10] have been successfully entrapped. However, in these cases the primary event (that is, ligand binding) was not coupled to a downstream physiological process, and thus the materials did not show full biochemical functionality.

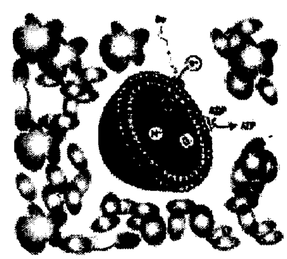
The work by Dunn and colleagues is the first to demonstrate the formation of stable chemical gradients across entrapped membranes, and more importantly, to show that the presence of the gradient can be used to drive biochemical synthesis (Fig. 2). The authors entrap liposomes that contain the transmembrane protein bacteriorhodopsin, which has the physiological ability to generate light-induced transmembrane proton gradients. Using a

pH-sensitive fluorescent dye located in the interior aqueous compartment of the liposome, the authors are able to demonstrate the formation of stable proton gradients across the membrane, which has the effect of 'storing' the light energy. By including a second membrane-associated protein, F_0F_1-ATP synthase, in the proteoliposome, the photo-induced proton gradient can be used to initiate the biosynthesis of ATP. The ability to 'store' the light energy as ATP has the advantage of eliminating passive leakage of ions across the membrane, but more importantly the use of ATP as a storage medium guarantees that many important biological processes could be powered by this storage cell. Hence, such materials could serve as biosolar cells or solar-based biofuel cells. Further, because the energy is stored as ATP, the use of the material for direct powering of motor proteins could allow conversion of the chemical energy of ATP to mechanical energy.

Fig. 2

Figure 2 | **Membrane-protein architecture in a silica pore, with the chemical events of proton pumping and ATP synthesis shown.**

Bacteriorhodopsin (shown in orange) absorbs a photon of light, causing protons to be pumped across the bilayer lipid membrane to the interior of the liposome. The proton gradient activates F_0F_1-ATP synthase (shown in yellow), causing conversion of ADP to ATP.



Although these biocomposite materials clearly have significant potential for power generation, a key issue that remains to be explored is the long-term stability of the entrapped membrane proteins. The chemical structure of sol–gel-derived biomaterials evolves over periods of several months as continued hydrolysis and condensation of silica occur. This leads to slow changes in pore morphology and silica surface chemistry, which can ultimately lead to a reduction in protein activity. Further advances in sol–gel processing are likely to be needed to better control material stability.

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Education

University of California, Los Angeles (Los Angeles, CA)

- Ph.D. in Biomedical Engineering, January 2005
  Major: Hybrid Bio-nanotechnology, Molecular and Cellular Bioengineering
  Minors: Microelectromechanical Systems (MEMS)/ Mechanics of Motor Proteins
  Dissertation: *Fabrication and Characterization of Biomolecule-Copolymer Hybrids as Energy Conversion Systems*

- M.S. in Biomedical Engineering, June 2003
  Thesis: *Hybrid* ***Protein*** */ Polymer Biomimetic Valves*

- B.S. in Physiological Sciences, December 2001
  Undergraduate Research Project: *Rapid Bacterial Diagnosis-MEMS-based DNA/RNA Detection*

Academic Positions

2005-Present
Research Associate

- **California Institute of Technology (Caltech)**
  Department of Bioengineering/Electrical Engineering
  Mentor: Professor Yu-Chong Tai

Research Topic: Using nano/micro technologies and bio-cloaking materials for improving biocompatibility and enhancing of implant efficiency

2005-Present
California Nanosystems Institute/Hewlett-Packard Postdoctoral Research Fellow

- **University of California at Los Angeles (UCLA)**
  Department of Mechanical Engineering
  Mentor: Professor Yong Chen (Top 50 Nanotechnologist in the United States-Scientific American)
  Research Topic: Interfacing nanofabricated electrode arrays with neurons and cardiomyocytes for nanoscale interrogation applications

Research Interests

- Integrate **protein**-functionalized copolymeric membranes with nano/MEMS technology
- Investigate energy conversion and production from motor proteins and membrane integration
- Study the interfacial bio-mechanical interactions between **cell** and Copolymer-Collagen thin substrate films
- Improve biocompatibility through bio-cloaking materials

Publication

- **D. Ho**, B. Chu, H. Lee, and C.D. Montemagno, "**Protein**-driven Energy Transduction Across Polymeric Biomembranes," *Nanotechnology* **15** (8), 1084-1094, 2004. See *Nature Materials (News),* July 8, 2004. ***Article downloaded over 1000 times; top 10% of all Institute of Physics (IOP) Publications (Information as of July 2005).***

- **D. Ho**, B. Chu, J.J. Schmidt, J., Brooks, E., Montemagno, C.D., "Hybrid **Protein**/Polymer Biomimetic Membranes," *IEEE Trans. Nanotechnology*, **3** (2), 256-263, 2004.

- **D. Ho**, and C.D. Montemagno, "The Advent of Innovation-Societal Perspectives of the Integrative Nanotechnology Revolution," published online at Institute of Physics website, www.nanotechweb.org; published online, *Nanotechnology*, 2005.
- J. Xi, **D. Ho**, B. Chu, and C.D. Montemagno, "Lessons Learned From Engineering Biologically-Active Hybrid Nano/Micro-devices," *Advanced Functional Materials* **15** (8), 1233-1240, 2005. ***Feature Article***

- **D. Ho**, B. Chu, H. Lee, E.K. Brooks, K. Kuo, and C.D. Montemagno, "Light-Dependent Current Generation Based on Coupled **Protein** Functionality," accepted *to Nanotechnology*, December 2005 as ***Cover Article***

- **D. Ho,** A. Fung, and C.D. Montemagno, "Engineering Novel Diagnosis Modalities and Implantable Cytomimetic Nanomaterials for Next Generation Medicine," accepted to *Biology of Blood and Marrow Transplantation*, 2005. ***Invited Paper***

- **D. Ho,** D. Garcia, and C.M. Ho, "Using Advanced Nanomanufacturing and Characterization Modalities Towards the Realization of Bio-Nano-Informatics Systems," accepted to *Journal of Nanoscience and Nanotechnology*, 2005.

- **D. Ho**, D. Wendell, and C.D. Montemagno, "Developing Hybrid Bionanosystems Using Synthetic Biology," A chapter in **The Springer Handbook of Nanotechnology**, accepted April 2005. (Includes contributions by Gerd K. Binnig, Winner of the 1986 Nobel Prize in Physics)

- D. Garcia, **D. Ho**, and C.M. Ho, "Bio-Nano-Information Fusion," A chapter in **Nanotechnology: Science, Innovation, and Opportunity,** accepted April 2005. (Includes contributions by Richard E. Smalley, Winner of the 1996 Nobel Prize in Chemistry; Mihail Roco, Director of the National Nanotechnology Initiative)

Sbumitted Publication

- H. Lee, **D. Ho**, and C.D. Montemagno, "Fluorometric Measurement of Vectorially-Inserted Purple Membrane Activity Across Block Copolymer Thin Films," Submitted to *Langmuir, 2005*

- **D. Ho**, S. Chang, and C.D. Montemagno, "Fabrication of biofunctional nanomaterials via *Escherichia coli* OmpF **protein** air-water interface insertion/integration with copolymeric amphiphiles," submitted to *Nanomedicine*, 2005.

- **D. Ho,** and Y. Chen, "Interfacing Cellular Systems with Abiotic Materials Using Composite Collagen-Block Copolymer Thin Films," submitted to *Nanotechnology,* 2005.

- **D. Ho**, and Y. Chen "Block copolymer-collagen Type I composite substrates induce alignment of C2C12 skeletal myoblasts," to be submitted to *Proceedings of the National Academy of Sciences-USA*, 2005
- **D. Ho**, and Y. Chen "Dexamethasone-Copolymer Composite Materials as Macrophage Anti-Inflammatory Materials for Enhancement of Implant Biocompatiblity." to be submitted to *Nature Materials*, 2005.
- **D. Ho**, B. Chu, H. Lee, K. Kuo, and C.D. Montemagno, " Enhancing Conversion Efficiencies of Light-Dependent Proton Pumps Using Quantum Dot Nanocrystals," in preparation, 2005.
- B. Chu, **D. Ho**, H. Lee, K. Kuo, and C.D. Montemagno, "Composite Proton Exchange Membranes Functionalized with Biomolecules Reduce Methanol Crossover and Electro-osmotic Drag," in preparation, 2005.

Conference Papers

- J. Huang, A. Shalchi, **D. Ho**, Y.H. Zhang, E. McCabe, and C.M. Ho, "Rapid Bacterial Diagnosis-MEMS-based DNA Detection," *Pediatric Research* **51** (4) 1610 Part 2 Suppl. (2002)
- **D. Ho**, J.J. Schmidt, and C.D. Montemagno, "**Protein**/Polymer Hybrid Biomimetic Valves," *Proceedings of the Materials Research Society,* **735** C.4.5.1-C.4.5.4 (2003)
- **D. Ho**, and C.D. Montemagno, "Hybrid **Protein**/Polymer Biomimetic

Membranes," *IEEE Proceedings on Nanotechnology* (1), 379 -382, August 2003

- H. Lee, **D. Ho**, J.J. Schmidt, and C.D. Montemagno, "**Biosolar** Powered Fabric," *IEEE Proceedings on Nanotechnology* (2), 733 -736, August 2003
- **D. Ho**, B. Chu, H. Lee, and C.D. Montemagno, "Directed **Protein** Adsorption by Site-specific Labeling," *IEEE Proceedings on Nanotechnology* (2), **Special Paper Session** Paper Suppl. 2003
- **D. Ho**, B. Chu, and C.D. Montemagno, "Nanoscale Hybrid **Protein**/Polymer Functionalized Devices," Proc. SPIE Int. Soc. Opt. Eng. **5389**, 192 (2004)

- **D. Ho**, B. Chu, K. Kuo, and C.D. Montemagno, "Functionalizing Biomimetic Membranes with Energy Transducing Proteins," *Proc. of the Mat. Res. Soc.* ***823***, W11.8.1-W11.8.6, 2004
- **D. Ho**, B. Chu, H. Lee, K. Kuo, and C.D. Montemagno, " Fabrication of Hybrid Bionanodevices Based on Coupled **Protein** Functionality," *Proc. ASME NANO*, Pasadena, CA September 22-24, 2004
- **D. Ho**, B. Chu, H. Lee, K. Kuo, and C.D. Montemagno, " Electrochemical Measurement of Coupled **Protein** Functionality Across Polymer Membranes," Accepted to *Proc. Electrochem. Soc.- Intl. Symp. on Nanoscale Devices, Materials, and Biological Systems: Fundamentals and Applications*, Vol. AH1, 2004

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- H. Lee, **D. Ho**, B. Chu, K. Kuo, and C.D. Montemagno, " Reconstituting Biomolecules into Artificial Membranes and Detection of their Activities," *Proc. ASME NANO*, Pasadena, CA September 22-24, 2004

- H. Lee, **D. Ho**, B. Chu, K. Kuo, and C.D. Montemagno, " Membrane Proteins in Artificial Systems," Accepted to *Proc. Electrochem. Soc.- Intl. Symp. on Nanoscale Devices, Materials, and Biological Systems: Fundamentals and Applications*, Vol. AH1, 2004.
- **D. Ho**, B. Chu, H. Lee, K. Kuo, and C.D. Montemagno, "Synthesis and Characterization of Biomolecular Hybrids as Energy Conversion Systems," *International Symposium on Environmental Nanotechnology 2004*, Taipei, Taiwan, December 1st, 2004.
- **D. Ho**, B. Chu, H. Lee, K. Kuo, and C.D. Montemagno, "Coupled-**Protein** Functionality for Energy Conversion in Biomimetic Systems," accepted to *IEEE Robio Conference*, Hong Kong, June 28-July 3, 2005.
- **D. Ho**, B. Chu, H. Lee, K. Kuo, E.K. Brooks, and C.D. Montemagno, "Light-Dependent Current Production Using Biofunctional ABA Triblock Copolymers," *Bio-Nano-Information Fusion*, Marina Del Rey, California, July 20, 2005.

- **D. Ho**, and Y. Chen, "Interfacing Cellular Systems with Abiotic Materials Using Composite Collagen-Block Copolymer Thin Films," *Bio-Nano-Information Fusion*, Marina Del Rey, California, July 20, 2005.

- **D. Ho**, and Y. Chen, "Induction of Muscle **Cell** Alignment Using Copolymer-Collagen Type I Biofilms Possessing Relative Stiffness Gradients." submitted to *Proc. of the Mat. Res. Soc.* October 2005.

- **D. Ho**, and Y. Chen, "Diblock Copolymer Amphiphiles as Nanoscale Buoys for Interfacial Deposition of Collagen Type I." submitted to *Proc. of the Mat. Res. Soc.* October 2005.

- **D. Ho**, E. Chow, G. Cheng, and Y.C. Tai, "Dexamethasone-Triblock Copolymer Composites as Immune-Suppressing Materials for Enhancement of Implant Biocompatiblity." submitted to *Proc. of the Mat. Res. Soc.* October 2005.

Invited Seminars

- "Hybrid Nanotechnology," Bionanotechnology: Academic and Industrial Partnerships in the UK and US, University of Southern California, June 10th, 2004
- "Fabrication of Biomolecule-Copolymer Hybrids as Energy Conversion Systems", California Nanosystems Institute (CNSI) Invited Talk, University of California, Santa Barbara, February 18, 2005
- "Light-Dependent Current Generation from Biofunctionalized ABA Triblock Copolymers," Academia Sinica, Taipei, Taiwan, June 22, 2005.

- "Realizing Cytomimicry Through Biotic-Abiotic Interfacing," Keck Graduate Institute Special Seminar, Claremont, CA Nov. 3rd, 2005.

International and National Conference Presentations

- D. Ho, J.J. Schmidt, E.K. Brooks, and C.D. Montemagno, Engineering Pore Proteins as Nanoscale Microfluidic Valves, *NM2- Conference on Molecular Mechanics*, **Scholarship Recipient**, Poster Presentation, Maui, HI, May 12-17, 2002
- D. Ho, J.J. Schmidt, E.K. Brooks, and C.D. Montemagno, Engineering Pore Proteins as Nanoscale Microfluidic Valves, *California Nanosystems Institute (CNSI) Poster Symposium,* 2002
- D. Ho, B. Chu, J.J. Schmidt, E.K. Brooks, and C.D. Montemagno, "Engineering Pore Proteins as Nanoscale Macromolecule Sensors", University of California Systemwide Bioengineering Symposium, San Diego, CA, June 21-23, 2003. **Best Poster Presentation Award Winner**
- D. Ho, B. Chu, and C.D. Montemagno, "Nanoscale Hybrid **Protein**/Polymer Functionalized Devices," SPIE Meeting on BioMEMS and Nanotechnology. March 2004.
- D. Ho, B. Chu, H. Lee, and C.D. Montemagno, Functionalizing Nanoscale Polymeric Biomimetic Membranes with Energy Transduction Proteins, *CESASC Annual Convention*, May 22, 2004.
- D. Ho, B. Chu, H. Lee, and C.D. Montemagno, "Synthesis and Characterization of Biomolecule-Copolymer Hybrids as Energy Conversion Systems," *CESASC Annual Convention*, April 22, 2005.

Fellowships and Awards

- Faculty Woman's Club Endowed Scholarship, 1997
- Guenther Empowerment Award, UCLA Unicamp 1999
- UCLA Chancellor's Service Award, 2002
- University of California, Los Angeles, Bioengineering Dept., Departmental Fellowship, 2002-2003
- DARPA Molecular Mechanics Scholarship Winner, 2001 (for poster presentation)
- Best Poster Presentation Award Winner, UC Systemwide Bioengineering Symposium, 2003
- University of California, Los Angeles, Bioengineering Dept., Departmental Fellowship, 2004-2005
- Full Member, Sigma Xi Research Society, elected Fall 2004
- Dr. Denny J. Ko Future Entrepreneurs Scholarship, Spring 2005

Professional Memberships

- Materials Research Society
- American Society of Mechanical Engineers (ASME)
- Society for Optical Engineering (SPIE)
- American Association for the Advancement of Science (AAAS)
- Founding Member, American Academy of Nanomedicine
- Full Member, Sigma Xi Research Society (Elected)
- Member, Biomedical Engineering Society (Elected)
- Institute of Electrical and Electronics Engineers, Inc. (IEEE)

Community Service and Activities

- President, Vice President - UCLA Interfraternity Council, 2000-2002
- President - UCLA Pi Kappa Phi Fraternity (2 year term), 1998-2000
- External Vice President-Engineering Graduate Students Association, 2002-2003
- Founder- First Annual UCLA Dance Marathon, 2001
- UCLA Unicamp Head Counselor and WALL advisor, 1998-Present
- Member – Chancellor's Service Award Selection Committee, 2001

PHYSICAL CHEMISTRY 1

CHEMICAL CENTRE, SCIENCE FACULTY

LUND UNIVERSITY, SWEDEN

ANNUAL REPORT 1999

Cover:

AFM images of two-dimensional single crystals of C24 ceramide III in cholesterol monolayers (ceramide:cholesterol molar ratio 1:0.4, 1:1 and 1:2 respectively). The ceramide crystals are ca 0.8 nm thicker than the surrounding phase. Image size 2¥2 mm.
(E. Sparr, K. Ekelund, L. Eriksson)

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Ali Khan Fredrik Joabsson

2

Surface Chemistry and told me that my technique would be ideal for studying ionic interactions, so important for the surfactant systems they had developed. For the younger generation it may be mentioned that Ekwall is the pioneer of surfactant research in Scandinavia (and one of the leaders world-wide); when I met him he was 70 and had on his retirement as professor from a Finnish university, Åbo Akademi, a few years earlier started the laboratory in Stockholm, and made it into an important center. The next day, I visited his institute and met his coworkers, Leo Mandell and Krister Fontell and made up plans for research on micellar solutions, different liquid crystals and microemulsions; it is interesting that Ekwall and Fontell being behind some of the pioneering and still central observations on microemulsions refused to use this word. Referring to thermodynamically stable solutions they found it a misnomer. (Some years later, Ingvar Danielsson, Krister Fontell and myself wrote a short paper to clarify the microemulsion concept; however, in the last minute Krister Fontell refused to be a co-author because for him everything had been clear already in his early papers.) During several coming years, in Stockholm and Lund, I performed collaborative work on several different systems with Ekwall and Fontell and learnt immensely on surfactant physical chemistry.

Sture Forsén, a favourite teacher during the undergraduate studies and showing more and more interest into my work, at the same time became (record-young) professor at the new Lund Institute of Technology (to become a Faculty of Engineering in Lund University). Under the circumstances it was easy to accept Sture Forsén's offer for first a part-time (commuting from Stockholm) teaching assistantship in Lund and then after some time full time and moving to Lund (and, in lack of experimental facilities in Lund, commuting back to Stockholm for research). In Lund, Sture Forsén in a short time created a new laboratory (Physical Chemistry 2) of highest international standard. In spite of his then different research interests, he offered unfailing support to the research on surfactants.

The new-started laboratory of Physical Chemistry 2 offered very different working conditions than what we offer now our PhD students, to the better and to the worse. For example, still a graduate student and teaching assistant, you were the second oldest in the department, and could, therefore, even at the age of 27, replace the professor and be deputy head and professor during his sabbatical leave. Also you had the privilege to take care of students for diploma work and even PhD students, still being a PhD student yourself. In this as in many other ways I was extremely fortunate: the first two summer students and diploma workers were Håkan Wennerström and Göran Lindblom. They were given the task to continue some of the preliminary work from Stockholm, Håkan on the interaction between halide ions and hydrophobic ions and Göran on ion binding in surfactant systems. Work on ion binding to proteins was started together with a biochemist (then still working on his PhD thesis) from Uppsala, Michael Zeppesauer (later Professor in Saarbrücken) while the work on polyelectrolytes was taken up some years later with a another PhD student, Hans Gustavsson.

Sometimes, mistakes helped us progress, like when I had asked Göran Lindblom to do 35Cl quadrupole relaxation on some liquid crystalline phases. The experimental approach was then to extract the transverse relaxation rate from the line-width of continuous-wave spectra. At first this worked well but one day he came with some very strange line shapes. Excluding experimental artefacts, there was a lot of worry until Håkan Wennerström found out that they were due to quadrupole splittings. To complicate matters, the splittings first obtained were of second order; thereafter, we could easily find the first order splittings and use them as a very powerful tool for studying ion binding in

lamellar and other phases.

Another of these special observations was when Nils-Ola Persson (a new PhD student) was to investigate the hydration in a special liquid crystalline phase, the "C phase", detected in Ekwall's group. In addition to the normal doublet, characterising an

enzyme) systems using different nuclei such as 23Na, 35Cl, 79Br, 25Mg, 43Ca, 85Rb and 127I. I came to a small department with research in inorganic solution chemistry (afterwards to be transferred to the Department of Inorganic Chemistry 1) and ample room for starting new activities. However, the building up of a problem-oriented research programme in the general field of colloid and surface chemistry, a very exciting and stimulating team-work together with many seniors now present at the department, is another story.

For me it thus started with temperature anomalies, but opportunities and coincidences brought me in other directions. Regarding the water anomalies, the great proponent was W Drost-Hansen, who had published a series of papers in the early and mid 60s which received a lot of attention. I did not follow this literature afterwards but by chance got to see many years laters a paper by Drost-Hansen which starts: "Various workers1-12 have reported the existence of thermal anomalies ("kinks") in the properties of bulk water and bulk aqueous systems" and later says "thermal anomalies .... at a number of discrete temperatures". However, on the basis of the new results and reconsidering previous ones he concludes: "The results of the present study suggest no evidence whatever for the reality of such anomalies" and "there is no evidence for the existence of thermal anomalies". When Drost-Hansen's paper was submitted for publication I had given up the water anomaly project and was already finishing my first paper on NMR studies of ion binding in surfactant systems.

Björn Lindman

Young Björn Lindmann (middle), flanked by Sture Forssén (left) and Göran Lindblom (right).

AFM images of mixed lipid monolayers. Left: Two-dimensional crystals of C24 ceramide III and C16 ceramide III in a cholesterol rich monolayer. Right: Addition of lignoceric acid (C24:0) to the previous mixture. Here, the regular shape of the domains is lost while the lateral arrangement is retained.

low q scattering from the smaller droplets. This allowed us to follow the growth of the bigger drops, even though the number ratio of big to small droplets is as low as 10-6. The nucleation process can be analysed in detail with knowledge of equilibrium properties. In another series of experiments, relaxation processes in sponge phases were studied by temperature-jump technique. In those experiments, we found that the relaxation rate (of the light scattering intensity) increases dramatically with increasing concentration. (A. Evilevich, T. Le, U. Olsson, H. Wennerström; P. Schurtenberger (Zurich), S. Egelhaaf (ILL, Grenoble), R. Strey (Köln)).

Thermodynamics of fluid surfaces. The L3 (sponge) phase and the balanced microemulsion are two phases that appear in binary and ternary surfactant systems. Both are disordered fluid membrane phases in which a topologically complex bilayer (L3) or monolayer (balanced microemulsion) separates two solvent domains. The thermodynamics of both phases have been modelled using an extended correction to the ideal scaling law typically used for infinite membrane phases. With this extension, we can capture thermodynamic features commonly found in both phases. "narrowness" in experimental phase diagrams and characteristic sequences of phase transitions. Ternary systems containing nonionic surfactants are particularly useful model systems for investigating fundamental properties of microemulsions and sponge phases due to the convenient temperature-dependence of the surfactant monolayer spontaneous curvature. We have investigated one such system, the C12E5-water-decane system, in great details and found that it is possible to obtain self-consistent interpretation of the phase equilibria of the sponge phase, balanced microemulsion and droplet microemulsion phases, and light scattering data of the sponge phase using the aforementioned elastic curvature model. (T. Le, U. Olsson, H. Wennerström, P. Schurtenberger (Zürich)).

Domain formation in lipid monolayers. Langmuir-Blodgett monolayers of mixed lipids is studied by means of surface pressure-area isotherms and AFM. Domain formation due to lateral phase separation is observed at different lipid compositions and surface

Alternative surfactants. Industrial interest continues in novel, especially biodegradable, surfactants like alkyl polyglucosides synthesised from renewable sources. Little research has been devoted to these systems. Phase diagrams, aggregate structure and microemulsion formation with model, and industrial compounds are investigated in co-opertion with Akzo Nobel. The aim is to identify molecular factors that govern the phase behaviour and so facilitating design of applications. Solution properties of an acyl-N-methylglucamide and an ethoxylated fatty acid amide are also under exploration. (A. Khan, U. Olsson, J. Reimer, O. Söderman, C. Whiddon, I. Johansson (Akzo Nobel)).

Structure of lamellar phases. The equilibrium structure and phase equilibria of the lamellar phase are sometimes complicated as noted in early studies by Ekwall and Fontell. This complication appears to be related to the formation of liposomes (onions) under shear, which can originate simply by shaking the sample. A systematic study was performed on nonionic surfactant-water systems where the structures of the lamellar phase under shear (Couette flow) was investigated using small angle scattering. Depending on the temperature, which governs the monolayer spontaneous curvature, we can identify two distinct regions corresponding to onions (lower temperature) and planar bilayers (classical lamellar phase, higher temperature). The equilibrium structure at zero shear, however, appears to be the classical lamellar structure. (T. Le, U. Olsson, H. Wennerström, K. Mortensen (Riso), Walter Richtering (Freiburg) and Johannes Zipfel (Freiburg)).

Emulsions. NMR techniques are used to study oil-in-water and water-in-oil type emulsions with varying volume fractions. Self-diffusion data show that molecules of the dispersed phase undergo a restricted self-diffusion whereas unbounded diffusion is the rule for the dispersion medium. The self-diffusion data can be used to determine emulsion characteristics such as droplet size, size distribution and interdroplet interactions. This project has focussed on NMR-methods for determining emulsion droplet sizes. Special emphasis is given to systems where other techniques fail In a related project new methods that allow the study of high internal phase ratio emulsions (concentrated emulsions) by means of the NMR self-diffusion approach have been developed. To interpret echo-decays observed in such systems we have developed a method based on Brownian dynamics simulation of molecules enclosed in cavities. The method gives information on droplet sizes and life times of molecules in the droplet. Extensions to include double emulsions of the w/o/w type, show that the NMR method yields important structural information. Concentrated emulsions are also being used as model systems in developing methods to study a class of porous media by means of pulsed field gradient NMR. In particular the new method of modulated field gradients is being used in the study of such emulsions. (B. Håkansson, M. Nydén, P. Linse, O. Söderman).

Non-ionic surfactants as solubility enhancers in pharmaceutical formulations. Aqueous formulations comprising hydrophobic drug molecules often require the use of solubility enhancers that increase the concentration of the active substance to therapeutically acceptable levels. Traditionally, PEG based surfactants have been used for this purpose. These surfactants have, however, certain pronounced draw-backs, most importantly a low long-term chemical stability in aqueous solution. Furthermore, many degradation products of PEG (e.g. formaldehyde and formic acid) are toxic. Within the present project, sugar based surfactants are studied as potential alternatives to PEG based surfactants in pharmaceutics. The investigations include characterisation of non-ionic micellar systems by spectroscopic and

corresponding decrease in the viscosity, was found with increasing shear rate at high block copolymer concentrations. At low polymer content, however, the samples were shear thickening, and a shear-induced formation of multilamellar vesicles (onions) was observed. The influence of polymer concentration, block length and solvent composition on the behavior under shear are investigated (project completed). (P. Alexandridis, M. Tsianou, G. Schmidt, J. Zipfel (Freiburg), W. Richering (Freiburg)).

Amphiphilic block copolymers in selective solvent. A combined experimental and theoretical study of the phase behavior and the structure in binary and ternary systems of block copolymers in selective solvents has been made. The block copolymers considered are poly(ethylene oxide)-poly(propylene oxide) - poly(ethylene oxide) and the solvents are water and xylene. This is the first time a reverse (water-in-oil) hexagonal phase has been observed for a PEO-PEO-PEO/water system, and moreover this is also the first report that a given amphiphile/water system displays both a normal (oil-in-water) hexagonal and reverse hexagonal phase at the same temperature. A mean-field lattice theory was used to predict phase diagrams and structural results of, in particular, the lamellar phase of the binary and ternary systems. The model predicted stability ranges of disordered solutions and lyotropic liquid crystalline phases at increasing PEO-PEO-PEO concentration in good agreement with experimental results. Moreover, the model provided volume fraction profiles for the PEO, PPO, and water components in the self-assembled structures. Regarding the ternary systems, phase diagrams for different PEO-block lengths of the PEO-PEO-PEO block copolymer have been predicted, and a detailed description of the domain spacing and interfacial area per PEO block as well as the chain conformation has been obtained (project completed). (M. Svensson, P. Alexandridis, P. Linse).

Block copolymer vesicles in dilute aqueous solution. The project involves the investigation of block copolymer vesicles and their stability in aqueous solution. The block copolymer used is a triblock copolymer of poly(ethylene oxide) and poly(propylene oxide), (PEO-PPO-PEO). Unilamellar vesicles are formed from dilute solutions of dispersed lamellar phase of the block copolymer. The experimental techniques employed are cryo-TEM and dynamic light scattering. These block copolymer vesicles may be stabilized, electrostatically or sterically, by the addition of single- or double-chained surfactants or polymers. (K. Schillén, K. Bryskhe, Y. S. Mel'nikova).

Interactions between starch and hydrophobically modified polymers. Amylose can form inclusion complexes where the hydrophobic tails of surfactants and lipids are included in the amylose helix. We have found evidence for a similar complexation between amylose and a hydrophobically modified polymer (HMHEC). Even small amounts of added amylose give rise to a marked viscosity increase for semidilute solutions of HMHEC, but not for non-modified HEC. The viscoelastic "gels" formed in the mixed solutions are thermoreversible. Small amounts of added surfactant destroys the amylose-HMHEC complexation by competitive association to HMHEC and, presumably, also by complexation between the surfactant and amylose (M. Egermayer, I. Chronakis, L. Piculell).

Effects of polymers on adhesion formation in surgery. Adhesion formation is a well-known complication of abdominal and pelvic surgery. Together with Stig Bengmark and Kåre Larsson (Ideon research Center) and Lena Holmdahl (Östra Hospital, University of Göteborg) we investigate the effect of water-soluble polymers and find very significant effects with

Polymer-Surfactant Systems

Polymers in vesicle solutions. Vesicles composed of oppositely charged surfactant mixtures (catanionic vesicles) can be prepared with controlled size, polydispersity and stability. Both cationic- and anionic-rich vesicle phases occur at the water apex of the phase diagram of these mixtures, allowing control of aggregate charge. Catanionic vesicles in the system SDS-DDAB-water have been characterised by means of direct imaging using cryo-TEM and optical microscopy, and by NMR Self-Diffusion. The effect of polymer addition on vesicle structure and stability is being investigated; and phenomena at high polymer addition like phase separation and gel formation. The polymers used are polyelectrolytes and nonionic polymers, both unmodified and hydrophobically modified. These are added to the SDS-rich and DDAB-rich vesicle solutions. With cationic polyelectrolytes JR400 and LM200 (HEC derivatives, the latter being hydrophobically modified) and anionic-rich vesicles, at very low degree of charge neutralisation, the polymer affects the structure of the vesicle suspension considerably. Ultimately it induces phase transition (precipitate formation). At high polymer concentration, when the system undergoes charge reversal, a gel phase area forms. A bilayer structure (vesicles, discs and lamellar sheets), is revealed by cryo-TEM. These structural changes play an important role in the macroscopic (rheological) properties of the network. Other polymer-vesicle systems are under investigation. (A. Khan, B. Lindman, E. Marques, M.-G. Miguel (Coimbra), O. Regev (Beer-Sheva)).

Vesicle formation and stability. In recent years, there has been a considerable interest in using vesicles made of long double-tailed cationic synthetic amphiphiles (e.g., dimethyldialkylammonium halides and dialkylphosphate acid esters) as vehicles for gene delivery and as membrane model systems. However, the physicochemical properties of these vesicles are still not well characterized. Size, polydispersity, thermotropic phase behavior, surface potential, permeability, and physical stability of vesicles generally depend on the preparation protocol and on the physical conditions in the bulk solution. Our objective here is to examine the effects of vesicle preparation method, concentration and counterion of the amphiphiles, temperature, and additives on vesicle formation and physical (thermodynamic and colloidal) stability. We also examine the addition of surface polymers as steric stabilizers for cationic vesicles. This study includes techniques such as differential scanning calorimetry, isothermal titration calorimetry, cryo-TEM and scattering techniques. (P. Barreleiro, G. Olofsson, E. Feitosa (IBILCE/UNESP, Brazil)).

Hydrophilically modified hydrophobic polymers. We have synthesised a **copolymer** with a backbone of poly(dodecylmethacrylate) onto which hydrophilic poly(ethylene oxide) side-chains are grafted. The **copolymer** is insoluble both in water and oil (cyclohexane or isooctane), but it is soluble in water-in-oil microemulsions based on oil, AOT and water, where it gives rise to a substantial increase of the viscosity. Very large viscosity enhancements (> 103) can be obtained for large droplets and high (3%) polymer concentrations. Fluorescence studies show that the sizes of the microemulsion droplets are affected by the polymer. Studies by nmr self-diffusion and light scattering (dynamic and static) show that the mixtures contain droplet-**copolymer** clusters in equilibrium with a large fraction of "polymer-free" droplets. The cluster sizes depend on droplet size, droplet-polymer ratio, and the overall contents of polymer and droplets. When a homogeneuos mixture is diluted by oil, the fraction of polymer-bound droplets decreases. This eventually results in a loss of solubility of the **copolymer**. (A. Holmberg, L. Piculell, U. Olsson, P. Schurtenberger (Fribourg)).

surfactant molecules in EHEC gels is markedly non-Gaussian, presumably reflecting the considerable inhomogeneity of a chemically cross-linked gel. (J. Sjöström, H. Ashbaugh, L. Piculell, P. Hansson, O. Rosén, M. Nydén).

Hydrogel-Surfactant Interactions. We are examining the role surfactant and gel charge play on their interaction in two projects. In the first project we are studying the interaction of lightly cross-linked sodium polyacrylate (c-PA) with a mixed surfactant solution of DoTAB and C12E8. The charge of the surfactant solution in contact with the gel is tuned by varying the proportion of DoTAB to C12E8. The binding of DoTAB to c-PA is measured potentiometrically, and the deswelling of c-PA is measured gravimetrically. 1H-NMR measurements have been performed to determine the ratio of C12E8 to DoTAB in the bulk solution. We have found the binding of DoTAB and deswelling of the gel are only weakly affected by C12E8 , indicating that the interaction of the gel with surfactants is largely controlled by the net surfactant solution charge. In addition, the nonionic surfactant binds strongly to the gel in the presence of bound DoTAB. The interaction between C12E8 and c-PA is attributed to the presence of DoTAB micelles within the polymer network providing hydrophobic domains to which C12E8 can bind. Experiments are presently being prepared to examine the ordering of the mixed surfactant aggregates within c-PA using SAXS.

In the second project we are examining the interaction between dodecyl trimethyl ammonium chloride (DoTAC) and an amphoteric polyelectrolyte gel composed of anionic and cationic monomers. Gel charge is varied by changing the ratio of the anionic to cationic monomer. Preliminary measurements indicate that surfactant interactions with a polyampholytic gel are different than with a polyelectrolyte gel. While binding to the polyelectrolyte gel does not proceed beyond charge neutralization, the surfactant binds to the polyampholytic gel even after all the monomer charges have been satiated. The binding studies will be complimented with SAXS measurements and TRFQ studies in collaboration with Per Hansson at Uppsala University (H. Ashbaugh).

Gelation of steroid-bearing dextrans by surfactants. The interaction between dextrans hydrophobically modified by steroid groups and surfactants is investigated with respect to macroscopic properties and microstructure. While freshly prepared mixtures of the polymers with several surfactants do not gelify, a formation of stiff macroscopically tansparent gels is observed after several days in certain cases. Gelation is thermally reversible. Cryo-TEM shows a rod-like micellar structure of the surfactant. (A. Lopes, visiting scientist from ITQB, Portugal, B. Lindman).

Concentrated mixtures of oppositely charged polymer and surfactant. Here we revisit the phase behaviour of aqueous mixtures of sodium polyacrylate(NaPA) with cetyltrimethylammonium surfactants (CTAX; = Br, Cl, Ac), to investigate the structures and detailed compositions of the concentrated phases that separate out from such mixtures. Samples can be obtained with three macroscopically separated phases in equilibrium. The dependence of the phase behaviour on the global water content is best understood in terms of the concentration of the "simple salt" (NaX) which screens the attraction between the polyions and the surfactant aggregates. Polyacrylate ions not only bring the surfactant aggregates together, but also change their shape. Current studies take their departure in the truly ternary mixtures of the complex (CTAPA) salt with CTAX in water. A complete ternary phase diagram for CTAPA, CTABr and water has been established. Pure CTAPA swells in water, forming first a hexagonal and then a cubic phase. The hexagonal phase can be formed with arbitrary proportions of polymeric (PA) and monomeric (Br) anions, but the cubic phase is

Block copolymer-lipid interactions. The objective of this research project is to study the physical-chemical behaviour of a series of triblock copolymers of poly(ethylene oxide) (PEO) and poly(propylene oxide) (PPO) (PEO-PPO-PEO) ranging from water soluble to water insoluble in mixtures with lipids (lecithins) at room temperature. The present work focuses on 1) phase diagrams of mixtures between the more hydrophobic PEO-PPO-PEO copolymers (for example L121), lipid and water to investigate the miscibility of the different lamellar phases. 2) the dilute regime of the binary block copolymer system. 3) stability and kinetic studies of mixtures of the dispersed lamellar phase of lecithin and block copolymer. Methods, such as, small angle X-ray and dynamic light scattering and cryo-TEM are employed. (K. Bryskhe, K. Schillén, U. Olsson, J.-E. Löfroth)

Polymers labeled with fluorescent chromophores. Water-soluble polymers covalently labeled with fluorescent hydrophobic dyes have been synthesized and their solution properties are now investigated. The polymer is a polyelectrolyte, poly(acrylic acid) (PAA), and the chromophores are either pyrene or naphthalene, which are randomly attached onto the polymer. The aim is to achieve molecular understanding of the association processes in hydrophobically-modified polymer systems by using dye-labeled polymers. Fluorescence measurements (steady-state and time-resolved) combined with results from static and dynamic light scattering report on the self-association of the polymers in aqueous solution and also on their interaction with surfactants, other polymers or other additives. One study concerns, for example, the solution behaviour of dye-labeled PAA and the effects induced by added cationic surfactants in water. The time-resolved fluorescence measurements are to be performed in collaboration with Dr. J. P. S. Farinha, Lisbon, Portugal. (K. Schillén, B. Lindman, D. Anghel, M. da Graça Miguel

Protein-Amphiphile Systems

Protein-surfactant interactions in solution. The aim of the project is to investigate the protein-surfactant interactions in solution by following the phase behaviour of the systems over selected concentration range. Oppositely charged protein-surfactant pairs, such as, lysozyme-sodium dodecyl sulphate, ß-lactoglobulin-dodecyltrimethylammonium chloride (DOTAC), ovalbumin-DOTAC show a strong association and formed different phase regions. A novel gel phase, a large single solution phase and a two-phase region with a precipitate are characterised. Simple salts do not affect the general features of the phase behaviour but the alkyl chain lengths of the surfactants exert a strong effect on the stability of phases. A less rich phase behaviour is observed for the oppositely charged bovine serum albumin-DOTAC system which only exhibits a solution. The studies are extended to systems containing vesicles and lamellar liquid crystal forming surfactants, such as, Aerosol OT and didodecyldimethylammonium bromide.The microstructure of protein-surfactant complexes in solution and gel is investigated with techniques such as NMR and Cryo-TEM, AFM. (A. K. Morén, A. Stenstam, A. Khan).

Protein-lipid interactions. Studies on the relation between the lipid phase behaviour and protein-lipid interactions make use of cryo-TEM, X-ray scattering and different NMR techniques. Mixtures of ß-lactoglobulin (the major whey protein in milk, which is known to bind lipids) and phospholipid, are mainly investigated. The studies involve liquid crystalline (lamellar) phases, vesicle suspensions and the protein-lipid interactions at interfaces, e.g. emulsions. (J. Khakhar, T. Nylander, A. Khan; R. Bauer (Denmark); J. Skov-Pedersen (Denmark); M. Paulsson (Food Technology); E. Bylaite, R. Venskutonis (Lithuania).

Besides the experimental work, efforts are also made to describe the observed kinetics theoretically. A kinetic model has been developed in order to describe the kinetics of single and binary surfactant systems. (J. Brinck, B. Jönsson, F. Tiberg).

Surface forces in semi-dilute polymer solutions. By using the surface force apparatus (SFA) an attractive force with a long range was observed between macroscopic surfaces immersed in mixed semi-dilute solutions of dextran and poly(ethylene oxide). The range of the force (several thousands Ångstrms) exceeds the size of individual polymer coils by an order of magnitude. Thus, the range is much too long to be explained by classical depletion or bridging mechanisms. The formation of a capillary condensate between the two surfaces with a polymer composition different from the composition of the bulk solution was suggested to be the underlying mechanism. Despite that ethyl (hydroxyethyl) cellulose (EHEC) is a nominally single polymer system, which has been subject to extensive purification procedures, a similar force was found to operate also in semi-dilute solutions of EHEC. However, a recent separate investigation has shown that EHEC is a multi-component system that contains a range of chemically different polymer chains. The heterogeneity is believed to stem from the manufacturing process. In a similar way as in the dextran-poly(ethylene oxide) mixture, a surface induced segregation between different polymer fractions could be the origin of the long-range attractive force in the EHEC system. (H. Wennerström, K. Thuresson, T. Nylander, F. Joabsson, P. Linse, B. Lindman)

Interfacial properties of ß-casein. The interfacial properties and the structure of the adsorbed layers of a natural block copolymer, ß-casein, are extensively studied by ellipsometry, surface force measurements, and neutron reflectivity measurements as well as by applying a specific proteolytic enzyme, endoproteinase Asp-N. ß-Casein is a highly surface active protein from milk, which forms brush like structures at interfaces depending on the surface properties and the ionic strength and salt composition. The protein is extensively used as emulsifier and to stabilise colloidal suspensions. (T. Nylander, and F.Tiberg (YKI, Stockholm)).

Interfacial properties of wheat proteins. Various surface chemical techniques, like ellipsometry, surface film balance, and the surface force apparatus is used to study the interfacial interactions between pure fractions of the different wheat proteins. The interfacial properties and the interfacial interactions of the proteins are vital importance for the quality of wheats for use in food industry. (A.- C. Eliasson, J. Örnebro (Food Technology), T. Nylander).

Interacting forces between biological macromolecules. The interactions between salivary films adsorbed on mica surfaces are investigated using the interferometric surface force technique (SFA). Human whole saliva and purified fractions of saliva are used. These studies are of key importance for the understanding of intraoral events such as adhesion, friction and wear. Complementary neutron reflectivity measurements on the structure of the adsorbed layers have also been started.(T. Nylander, T. Arnebrant, P.-O. Glantz (Prosthetic Dentistry, Lund University) and F. Tiberg (YKI, Stockholm)).

Behaviour of hydrophobically modified polymers at surfaces. The adsorption of HMP(E)s at surfaces is investigated. Due to their amphiphilic nature HMP(E)s are potentially intresting for stabilising or flocculating particle and fibre systems. The project deals with the adsorption of different HMP(E)s at surfaces and the relation between their interfacial

produce stereo-images (3D) with a spatial resolution down to some nanometers. (K. Andersson, P. Barreleiro, J. Khakar, A. Khan, E. Marques, Y. Melnikova, A. K. Morén, S. Nilsson, K. Schillén, O. Regev (Beer-sheva), Y. Talmon (Haifa)).

Solution microstructure from NMR relaxation and self-diffusion measurements. NMR relaxation time and self-diffusion measurements, as applied to the study of microstructure in surfactant systems, have a long tradition in our department. A continuous development of theoretical models over the years have turned these experimental techniques into standard tools for investigating surfactant aggregate. Recently we have used this approach to investigate the solution microstructure in some oil-water-didodecyldimethylammonium surfactants with different counterions as well as to study the microstructure in surfactants forming bicontinuous micellar aggregates in a L1 phase. Self-diffusion experiments are used to investigate a viscoelastic microemulsion formed in the L2 phase of the lecithin-water-cyclohexane system. The structure is made up of giant reverse wormlike micellar aggregates. Combined measurements of water and lecithin self-diffusion behaviour gives information on structure and dynamics. For very long micelles we seem to observe the curvilinear lecithin diffusion along the micellar contour. By monitoring the time dependence of the mean square dependence we are able to obtain information on the micellar persistence length. Moreover, the methods have been used to characterize vesicle systems found in mixtures of cationic and anionic surfactants. Here, the method yields important information with regard to the presence of vesicles, their sizes and also to the dynamics of the surfactants. (U. Olsson, O. Söderman, A. Khan, E. Marques; M. Monduzzi (Cagliari), A. Ceglie (Bari), R. Angelico (Bari), G. Palazzo (Bari)).

Theory and Modelling

Temperature dependent dispersion forces. We are investigating the consequences for the dispersion forces of having a thermally excited radiation field. A number of conceptually important results follow. i) The asymptotic form of an atom-atom (or molecule-molecule) dispersion interaction is a potential varying as the inverse sixth power of the separation and not the inverse seventh power retarded interaction that is the present textbook result. ii) We find that generally the asymptotic form of the dispersion interaction is, on the free energy level, identical to the corresponding classical case, which amounts to a novel correspondence principle. iii) The mechanistic explanation of the so called retardation effects in terms of delays in a signal transmission seems misleading. (H. Wennerström, B. Ninham, J. Dacic (YKI)).

Diffusive transport in responsive media. We are studying molecular transport over a lamellar phase in the presence of a water gradient. Calculations are based on the interbilayer forces that induce swelling and phase transitions in respond to the variation in boundary conditions. Our model implies non-linear transport behaviours, due to the co-operative structural transformations along the water gradient. Water transport through a stack of lipid bilayers is also studied experimentally by a calorimetric technique and we find a pronounced break in the permeability when the relative humidity reaches the value of the liquid crystal to gel transition of the lipid. (E. Sparr, N. Markova, H. Wennerström).

Water and ions in aqueous solution. The efficiency of molecular dynamic simulations of water with polarizable potentials employing different boundary conditions has been examined. Moreover, the hydration of cations and anions with different polarizabilities was examined by Monte Carlo and molecular dynamics simulations for ions in bulk solution and in a water cluster. In particular, the solvation of the ion and the location of the ion in the cluster were found to depend on the charge and on the polarizability of the ion. (P. Linse; T. Nymand (Århus University), S. Brodarski and G. Karlström (Theoretical Chemistry, Lund);).

Statistical mechanical programs. Also during 1999 the statistical mechanical computer program MOLSIM for Monte Carlo and molecular dynamics simulation has substantially been updated and extended. For example, we have implemented routines (i) for Ewald summation of systems containing particles with charged, dipoles, and polarizabilities and (ii) for the so-called cluster move technique involving a simultaneous displacement of several nearby particles. The latter extension has dramatically increased our possibility to simulate charged colloidal solutions. (P. Linse; V. Lobaskin).

Micelle formation of block copolymers with charged blocks. Amphiphilic polymers as well as amphiphilic short chain surfactants tend to self-associate in solution. In the presence of charge, the possibility to regulate the self-association is increased by altering the salt-concentration and the pH in the case of titrating polyelectrolytes. We have extended the scaling analysis of these systems, and we have found a very rich appearance of different scaling regimes. Moreover, have also performed numerical lattice mean-field calculations to obtain complementary information such as volume fraction profiles, critical micellization concentrations and to examine when the asymptotic scaling regimes are valid. (P. Linse; N. Shusharina and A. Kohklov (Moscow)).

Amphiphilic block copolymers in selective solvent. Ternary poly(ethylene oxide)–poly(propylene oxide)–poly(ethylene oxide) (PEO–PPO–PEO)/water/oil systems have been studied theoretically with a lattice mean-field theory. Phase diagrams for three PEO–PPO–PEO block copolymers were determined, and the existence of the ordered cubic micellar, hexagonal, lamellar, reverse hexagonal, and reverse cubic micellar phases as well as disorded water-rich and water-poor phases was considered. It was found that the length of the EO blocks strongly affected the phase behavior. The lamellar phase was studied in more detail with respect to the domain spacing and interfacial area per PEO block at different compositions and to the polymer conformations. The degree of loop-like conformations and of bridging conformations across the apolar domain (PO + oil) was found to be dependent on the apolar domain thickness. (M. Svensson, P. Alexandridis, P. Linse).

Instruments Available At The Department

NMR (contact person: Olle Söderman). The department has a Bruker DMX200 NMR spectrometer, delivered towards the end of 1994. The spectrometer is well equipped and allows performance of a variety of modern NMR experiments, such as solid state experiments, advanced relaxation measurements and diffusion experiments. In addition, the department has at its disposal a Bruker DMX100 spectrometer, a Bruker MSL 100 spectrometer interfaced to a variable field electromagnet and a SMIS spectrometer interfaced to a JEOL 100 MHz electro-magnet. The latter system is a dedicated self-diffusion NMR spectrometer. (Sponsored by FRN and Kjell and Märta Beijers Stiftelse).

to the microscope and images are recorded, all under cryogenic conditions (liquid nitrogen

temperature). Other sample preparation methods availab' re for example freeze-fracturing and replica techniques. For traditional TEM, with solid st·re samples, the specimen is normally prepared by crushing the sample in a volatile solvent and dispersing it on to the hòley-carbon grid. For further in'ormation about the microscope see www.oorg2.lth.se/biomic/ (Sponsored by NFR, Crafoord Foundation and Knut and Alice Wallenberg-foundation).

Multimode scanning probe microscope (contact person: Emma Sparr). A Multimode Scanning Probe Microscope (Nanoscope-III) was purchased, with Sven Engström, Department of Food Technology, as responsible, from Digital Instruments Inc., Santa Barbara during April 96. The instrument performs both as a scanning tunnelling microscope (STM) and an atomic force microscope (AFM). With its many configurations the instrument can scan and image a wide variety of samples with scan sizes from atomic level up to 125 microns square. A liquid cell also allows this to be done in an aqueous environment. As an AFM it operates in either traditional contact AFM mode or TappingMode. In contact mode it produces topographical data and frictional data when operating as a lateral force microscope (LFM). The AFM mode also allows measurements of the interaction forces between the AFM tip, which can be modified, and the substrate surface. (Sponsored by FRN).

Optical Microscopy (contact persons: Ali Khan & Anna Stenstam). The Department has a Zeiss Axioplan Universal microscope equipped with differential interference contrast and a 35 mm photo camera MC 100 as well as with a 100W mercury short-arc lamp and a system of filters to allow the fluorescence microscopy observations. The microscope is further equipped with a high-sensitivity SIT video camera and an image processor, Argus 20. (Hamamtsu Photonics, Japan) together with the Macintosh-based image analysis software.(Sponsored by FRN & Crawford Foundation).

Light scattering (contact person: Lennart Piculell). For molecular weight characterisations and studies of conformation changes or association processes a modern light scattering instrument is available. The instrument is a Dawn F MALLS photometer (Wyatt Tech, Santa Barbara, California). This instrument is equipped with a 5 mW He-Ne linearly polarised laser. The intensity of the scattered light can be measured at 15 different angles simultaneously. It is possible to connect the instrument to a gel permeation chromatography system and on-line molecular weight determinations can be performed. The instrument can also be used for batch analysis, to obtain Zimm plots. (Sponsored by FRN) .

Polarimeter (contact person: Lennart Piculell). To measure conformational changes a Jasco DIP-360 polarimeter is used. The polarimeter can be thermostated to perform temperature sweep measurements.

Rheometer (contact person: Krister Thuresson). A Carri-med controlled stress rheometer CSL 100 temperature controlled by Peltier system. Measuring systems cone and plate (solvent trap) in acrylic (4 cm, 1° and 6 cm, 1°) and stainless steel (4 cm, 1° and 6 cm, 1°). (Sponsored by Nils and Dorthi Troëdsson Research Foundation).

UV-Vis spectrometer (contact person: Krister Thuresson). A Perkin Elmer lambda 14 UV/Vis is used to perform absorbance measurements (190-1100 nm). The spectrometer is

The program has a Board with industrial majority composed of the following members: Jan Svärd (Chairman; Akzo Nobel Surface Chemistry), Corne Bogentoft (Karolinska

Innovation), Ulf Carlsson (SCA Research), Kåre Larsson (Camurus), Bengt Nordén (Chalmers Institute of Technology), Karin Schillén (Lund University) and Per Stenius (Helsinki Institute of Technology). The host university of the Programme is Lund University; Programme Director is Björn Lindman and Programme Secretary Gerd Olofsson. Jan Christer Eriksson (Stockholm, S) was Director of Studies of the Graduate School during 1999. From the start of 2000, Krister Holmberg (Göteborg, G) has this position.

The research program is divided into 5 areas:

1. Dynamic surface forces (leader, Per Claesson,S).
2. Aqueous polymer mixtures and gels (Lennart Piculell),
3. Chemical reactions in organised media (Krister Holmberg, G).
4. Interfacial aspects of cellulose (Fredrik Tiberg, S), and
5. Concentrated dispersions (Ulf Olsson and Lennart Bergström, S)

During the end of 1997 we started to recruit Ph D students and by the end of 1999 19 students had been accepted; a few more have been accepted during the beginning of 2000.
3 courses (also open to students outside the program) were given during the year

- Surface and colloid chemistry- molecular basis and technological applications, Degeberga (22 participants)
- Phase equilibria and phase transitions in colloidal systems, Visby (37 participants)
- The colloidal domain, Stockholm, Göteborg and Lund (25 participants)

During the year there were 2 Board meetings, one in Lund and one in Göteborg. A Programme Workshop was arranged in Göteborg, hosted by SCA Research, with participation of the Board, the senior scientists, the Ph D students, and several representatives of Swedish industry and academic institutions. The Programme Workshop, which had more than 70 participants, consisted of plenary lectures, poster presentations of Ph D student projects and 3 parallel symposia. Two very successful international workshops were arranged, one on Oppositely charged polyelectrolyte complexes in Lund (together with Center of Amphiphilic Polymers) and one on Molecular interactions on cellulose surfaces in Sundsvall (together with Midsweden University). There were 70-80 participants in each event.

In 1999, the SSF Board decided on the total funding for the programme (to run until 2002) amounting to 64 MSEK.

Further information on the program (including the complete Programme Plan) can be found at the website of the program www.colintech.lu.se. A Midterm Report, in preparation, gives a detailed account of the activities. The e-mail address is colintech@lu.se

The Surface and Colloid Science Center. YKOLL,

our interdisciplinary center on surface and colloid science, held its 10th annual symposium on 20-21 October this year. As usual, the program contained an appealing blend of lectures, ranging from fundamendal to applied sciences, presented by a selection of "in-house" as well as external speakers. More than 30 posters (20 of which with authors from our department) illustrated the range of current projects within the area of surface and colloid science that are currently being pursued in Lund. There were this year 1[illegible] registered participants.

In conjunction with the Symposium, there was this year also a two-day Workshop on "Oppositely Charged Polymer/Colloid Pairs". The Workshop, which had 71 registered participants, was organised by Lennart Piculell and Per Linse as a joint activity of the Centre for Amphiphilic Polymers from Renewable Resources and the National Graduate School for

is to make a concerted effort to gain fundamental knowledge about the behaviour of whey proteins, relevant to improving methods of recovering them from whey and giving them the added value as food ingredients in the growing market for functional and probiotic foods. To

do this, a range of modern analytical, physical and theoretical methods will be applied to study whey protein (principally b-lactoglobulin) aggregation, gelation, denaturation and surface phenomena and the results will be interpreted using the growing body of molecular structural information. The project is coordinated by Dr Carl Holt, Hannah Research Institute, UK and apart from his institute and the Lund group (including Depts of Physical Chemistry 1, Physical Chemistry 2, Food Technology and Food Engineering) the other partners are: Mathematics & Physics, The Royal Veterinary and Agricultural University, Denmark; Netherlands Dairy Research Institute (NIZO); INRA Laboratory for Dairy Technology, France; Tecnología de los Alimentos, University of Zaragoza, Spain; Structural Biochemistry, University of Edinburgh, UK; Lab NMR CNR Institute of Macromolecular Chemistry, Milano, Italy; as well as the industrial partners Barculo Whey Products, The Netherlands; Armor Protéines, France; MD Foods, Denmark; Unigate plc, UK; Mestlé, Switzerland; Domo Food Ingredients, The Netherlands. Meetings within the project was held at Royal Danish Agricultural and Veterinary University, Copenhagen, Denmark March, 30-31 March, 1998, where Jan Khakhar gave a presentation, and in Arnhem, The Netherlands, September, 14-15- Tommy Nylander and Jan Khakhar participated in both meetings.

EU-Shared Cost Project.

A three year Shared Cost project entitled "Lipid-Lipase Structure Function Relationship: Novel Methods for Studying Interfacial Enzyme Actions and Relation to Structure of Self-assembled Lipid Nanostructures." (Contract no. BIO4-97-2365) was granted by the European Commision during 1997.

Production of lipases is an important industrial sector with applications in e. g. detergents, food processing, paper and pulp industry, leather preparation and speciality chemical industries. There is a continuous development of more effective and cost efficient products. The main efforts in exploring lipolytic enzymes has hitherto focused on the activity, the catalysis reactions using monomolecular substrates and the tertiary structure of the enzymes. However, it is known that the activity of the lipolytic enzymes is extremely dependent on the structure and the lateral organisation of the lipids, but the knowledge of the exact mechanisms of these interactions is very limited. Furthermore in industrial applications the mixing with the hydrolysis products, free fatty acids and di-and monoglycerides, as well as added surfactant molecules will alter the structure of the lipid aggregates as well as the characteristics of lipid/water interface.

Therefore this multidisciplinary project adopt a new approach to bridge the gap between the present knowledge of the binding of an individual substrate molecule and the interaction with "real" substrates, that is lipid aggregates (vesicles, micelles, emulsions, gels and liquid crystals). This means that we will consider the whole lipolytic process on the lipid aggregate level, lipid-aqueous interface and the enzyme 3D structure level.

The main aim of the proposal is to achieve more efficient lipolytic enzymes through:

a better understanding of the small-scale structure of lipid aggregates, which are important substrates for lipolytic enzymes

a better understanding of the influence of lipid structure on lipid-enzyme interactions

improvement of enzyme activity by protein engineering of the lipase.

Beside the main aim the proposed project will also determine the structure of lipid aggregates, which can be used as realistic substrates in new assays.

Chemistry, Uppsala University; Procter&Gamble Research Center, Kobe, Japan; Department of Physics, Kyoto University; Nagoya Institute of Technology, Japan; Shiseido Yokohama Research Center, Japan; Yokohama National University, Japan; Tokyo Metrpolitan University, Japan; Procter&Gamble Research Center, Brussels; Kao Tokyo Research Center, Japan; Institute for Surface Chemistry, Stockholm, Sweden; Royal Institute of Technology,

Stockholm; University of Gent, Belgium; Mitsubishi Chemical Corp., Yokohama; Tohoku University, Sendai, Japan; Japan Marine Science & Technology Center, Yokosuka, Japan; Pola Chemical Corp., Yokohama, Japan; Lion Corp. Research Center, Tokyo, Japan; National Institute of Materials and Chemical Research, Tsukuba, Japan; SCA Research Center, Sundsvall; Procter&Gamble Research Center, Cincinnati, Ohio; MidSweden University, Sundsvall; Chalmers Institute of Technology, Göteborg; Department of Physics, University of Minho, Braga, Portugal; Riga Technical University, Riga, Latvia; Björn Lindman was visiting professor at Department of Chemistry, Coimbra University, Portugal and Department of Physics, Kyoto University, Japan.

Håkan Wennerström was the invited Chairman for the Conference on Particles and Surfaces, Leyden. Håkan also attended the Meeting of the Portugese Chemical Society, Physical Chemistry Branch, Coimbra, and delivered a Plenary Lecture and visited Master Andrew of University of Manchester. Olle Söderman spent three months as a visiting scientist at the Water Research Institute in Tsukuba, Japan. Ingemar Wadsö gave an invited lecture at the Annual Meeting of the American Association of Pharmaceutical Scientists, New Orleans. Both Ali Khan and Johanna Borné gave oral presentation at the Conference. Lipase and Lipids: Structure, Function and Biotechnological Applications. Lennart Piculell and Per Linse were invited external expert participants at two-day internal workshop organised by Unilever in Liverpool, UK. Lennart visited at ESPCI, Paris; Copenhagen Pectin, Lille Skensved: SCA Research, Gothenburg; AstraZeneca, Göteborg; Akzo Nobel Surface Coatings, Stenungsund. Per attended The Ninham-Marcelja Symposium at Thorskogs Slott; hold two oral presentations at the 73rd ACS Colloid and Surface Science Symposiium, Boston; gave invited lectures at GelTex Pharmaceutical, Boston, at Structure of Charged Colloidal Suspensions workshop at University of Ljubljana, Ljubljana, at the Modelling of a Molecular Level workshop, Eka Chemicals, Bohus; presented two posters at the 4th Liquid Matter Conference, Granada, Spain. Per also visit the Department of Mathematics and Statistics, University of Melbourne, Australia, including an oral presentation and gave another oral presentation at PDC annual conference, KTH. Ulf Olsson was visiting scientist at Yokohama National University where he also presented a lecture. During the stay in Japan he also visited and presented lectures at Tokyo University, Tokyo Science University, Tokyo Metropolitan University, Japan Marine Science and Technology Center (JAMSTEC), Yokosuka, and Ajinemoto Company Research Centre, Kawasaki. He also visited Ochanomizu University in Tokyo and the reactor at the Tokai Research Establishment. Ulf Olsson also visited AstraZeneca Hässle, Mölndal, where he presented a lecture. Gerd Olofsson (local organizer) and Håkan Wennerström (member of the committee) organized Tenth Annual Surface and Colloid Science Symposium, at Kemicentrum, Lund. Almost all members of the department attended the symposium including a workshop on Oppositely Charged Polymer/Colloid Pairs which was organised by Lennart, Per and Gerd. All postgraduate students presented posters. Per Linse, Anna Stenstam, Marie Svensson also gave oral presentations on the workshop. Karin Schillén gave oral presentation at European Polymer Club Conference Breisach am Rhein, Germany, visited the Institute of Physics, University of Fribourg, Switzerland and Chalmers University of Technology.

Vladimir Lobaskin made two poster presentations at the 4th Liquid Matter Conference, Granada, Spain. Rouja Ivanova made oral presentations Nordic Polymer Days, Copenhagen;

Bengt Jönsson was one of the lecturers for the second chemistry course, and Eva Hansson, Lennart Piculell, Olle Söderman and Krister Thuresson were involved in leading exercises and question hours.

The topic of the third first-year course is thermodynamics and introductory quantum mechanics and spectroscopy. Olle Söderman is the head teacher for this course and shares the teaching with Bengt Jönsson.

As regards higher courses, the department gives one basic and one advanced course in surface and colloid chemistry. The basic course, which is a biannual event, is headed and taught by Ulf Olsson. As usual it attracts a lot of students (typically around 30) and is a popular course among the students!

The advanced surface and colloid chemistry course is organized and taught by Håkan Wennerström (main teacher) along with Lennart Piculell. It is given one a year during the fall semester, and is based on the book by Håkan Wennerström and Fennel Evans. It was offered for the first time during 1999 and attracted 8 students. Håkan organised a Ph. D. course on phase equilibria and phase transitions in Colloidal Systems at Fridhem Gotland and Håkan and Lennart were two of the five teachers for the course

The Institute for Surface Chemistry and YKOLL jointly organize an annual course on surfactants and polymers in aqueous solution directed towards an European audience. In 1999, the course was held in Lisbon, with Björn Lindman as one of the teachers. Björn Lindman also gave an advanced course on surfactant and polymer solutions at Coimbra University. was one of the teachers of the course - surface and colloid chemistry - molecular basis and technical applications for undergraduate and Ph. D students, arranged by the Colloid &Interface Technology Programme (SSF) in Degeberga, Sweden. Björn also lectured at different courses for industry in Sweden, Belgium, United States and Japan

Lennart Piculell gave a popular lecture on gels for high school (gymnasium) students visiting Lund University. Karin Schillen arranged tutorials on The Colloidal Domain-where Physics, Chemistry, Biology and Technology Meet; developed two lab exercises on the topic - light scattering and also lectured on scattering for the advanced course in Surface and Colloid Chemistry. Stefan Ulvenlund gave a lecture on - the surface & colloidal chemistry of pharmaceutics - for the second year course in physical chemistry.

FINANCIAL SUPPORT

For the fiscal year 1998/99 the department had a turnover of ca 28.0 million SEK, which is higher compared to the fiscal year 1997/98. From the University we obtained 9.83 million of which 2.27 million is to cover undergraduate teaching. 2.7 million, for graduate students; and 4.86 million to cover salaries of professors, associate professors (lektor) and assistant professor (forskarassistent), technical and administrative personnel, and basic expenses. Government research agencies that give support to the research are: The Natural Science Research Council (NFR), the Swedish Research Council of Engineering Sciences (TFR), which provide a support of, respectively, 6.6 million and [illegible] million SEK. The Swedish Board for Industrial and Technical Development (NUTEK) which supports more applied projects, supports us mainly via the Competence Center. during the year we obtained 3.0 million from NUTEK. We also received 5.3 million SEK from The Swedish Foundation for Strategic Research (SSF), which is an important funding agency for supporting novel research venture in Sweden. We are grateful for support from private industry, directly and via their foundations, amounting to ca. 1.0 million, and 0.6 million from The European Commission. In addition, we obtained ca 0.6 million from The Swedish Institute, foreign foundations, universities, industries. etc., to support Ph D students and postdoc projects, adjunct professor and short-term foreign guest scientists and for instruments etc.

May 7, 1999
Ström, Cecilia
Adsorption and Self-Assembly of Cationic Surfactants at Silica Surfaces.

Opponent: Prof. Johan Sjöblom,
Universitetet I Bergen, Norway.

May, 17, 1999
Suurkuusk, Malin.
Biophysical Studies of Apolipoprotein A-IM and a Partitioning Study.
Opponent: Prof. Kenneth P. Murphy,
University of Iowa, Iowa City, USA.

May 28, 1999
Håkansson, Björn
NMR self-Diffusion Studies of Surfactant and Polymer Systems. Methodology and Applications.
Opponent: Prof. Peter Stilbs, KTH,
Stockholm.

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Ioannis Chronakis, postdoc (Cranfield University, UK)
Marcel van Eijk, postdoc
Krister Eskilsson, forskningsingenjör

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Krister Thuresson, forskarassistent, (assistant professor)
Håkan Wennerström, professor

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Jan-Willem Benjamins
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Johanna Brinck
Karin Bryskhe
Malin Bydén *(jointly with Mid Sweden University, Sundsvall)*
Joakim Carlén
Fredrik Carlsson *(jointly with Institute for Surface Chemistry, Stockholm)*
Monica Egermayer
Jonny Eriksson *(jointly with Institute for Surface Chemistry, Stockholm)*
Krister Eskilsson
Alex Evilevitch
Katarina Flodström
Helen Gillgren
Yoshikatsu Hayashi
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Björn Håkansson
Philippe Ilekti
Jörgen Jansson
Fredrik Joabsson
Marie Jonsson
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Monduzzi, Maura, Universita di Cagliari (L)

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Effect of water soluble alcohols on surfactant aggregation in the C12E8 system.
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